

Regression Coefficient Example

Copyright 2022-2023 Battelle Memorial Institute

```
clearvars
load pnnl_napalm_data
```

Compute the regression coefficient matrices, B , for Classical Least Squares (CLS), Principal Component Regression (PCR), and Partial Least Squares (PLS).

```
[C_cls, B_cls] = pnnl_cls(A_train, C_train, A_unknown);
```

For PCR, use 3 principal components.

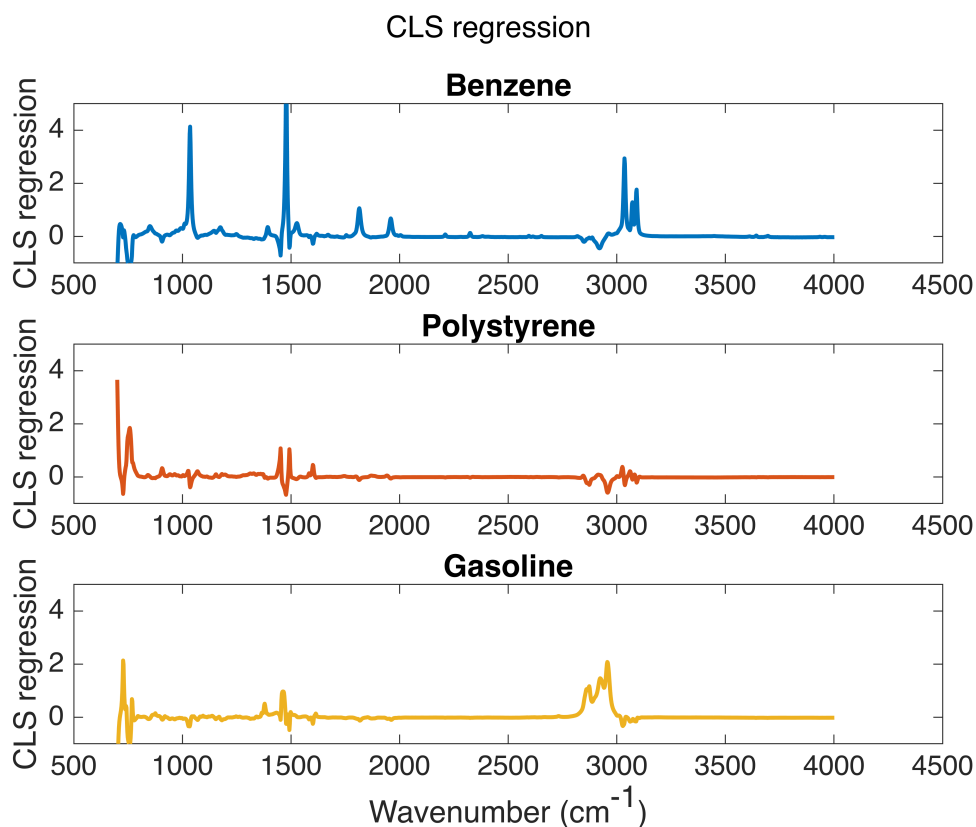
```
[C_pcr, B_pcr] = pnnl_pcr(A_train, C_train, A_unknown, 3);
```

For PLS, use 3 latent variables.

```
[C_pls, B_pls] = pnnl_pls(A_train, C_train, A_unknown, 3);
```

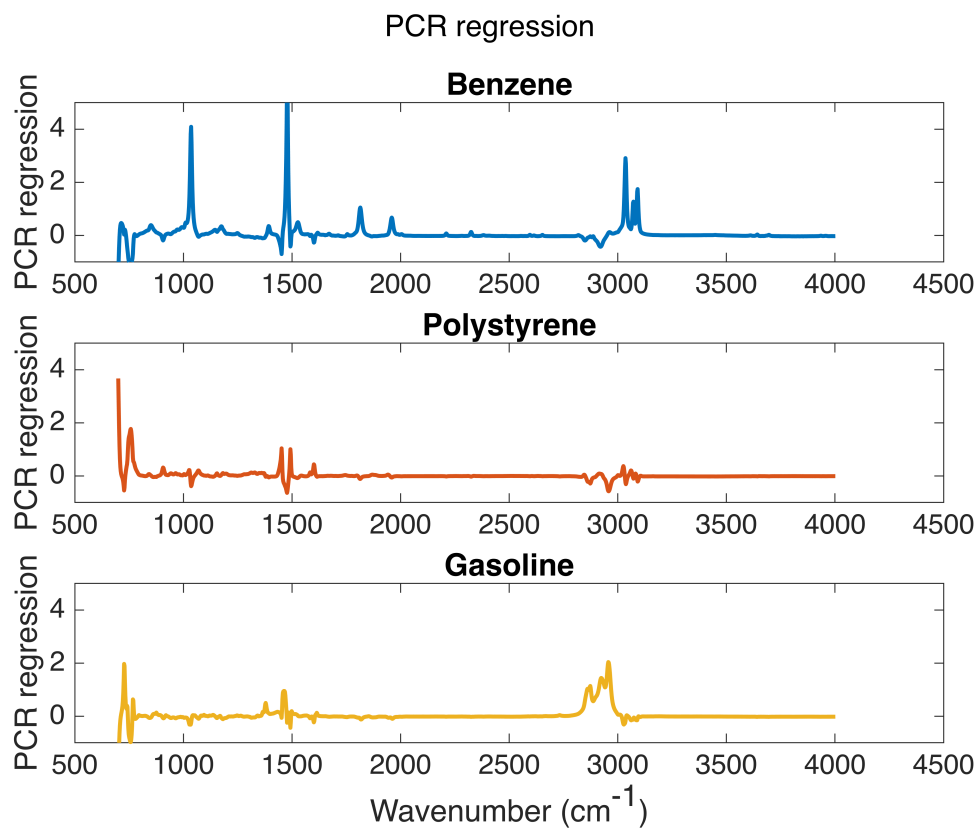
Plot regression coefficients for CLS.

```
plot_regression_coefficients(B_cls, 'CLS regression', Wavenumbers, WavenumberLabel, Consti
```



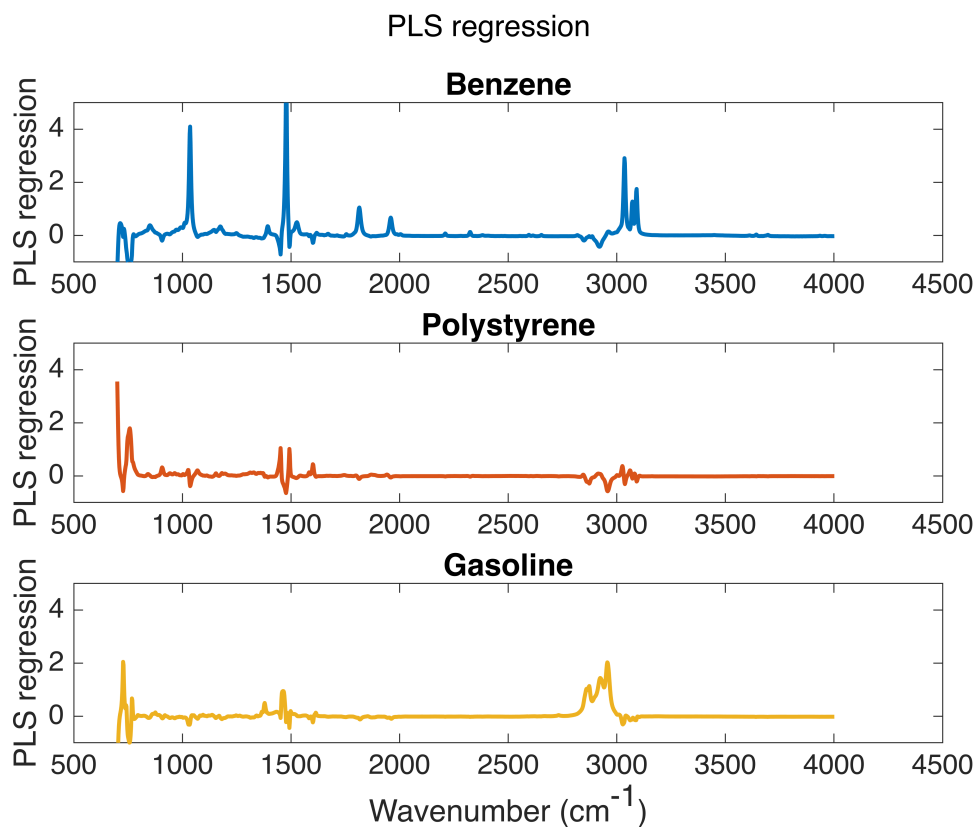
Plot regression coefficients for PCR.

```
plot_regression_coefficients(B_pcr, 'PCR regression', Wavenumbers, WavenumberLabel, Consti
```



Plot regression coefficients for PLS.

```
plot_regression_coefficients(B_pls, 'PLS regression', Wavenumbers, WavenumberLabel, Consti
```



```
function plot_regression_coefficients(B,y_label,Wavenumbers,WavenumberLabel,ConstituentNames)
figure
n = size(B,2);
colorOrder = pnnl_colorOrder(n);
figure;
h = gobjects(1,n);
for j = 1:n
    h(j) = subplot(n,1,j);
    plot(Wavenumbers,B(:,j),'LineWidth',2,'Color',colorOrder(j,:));
    title(ConstituentNames{j})
    ylabel(y_label)
end
sgtitle(y_label)
linkaxes(h)
xlabel(WavenumberLabel)
set(h,'FontSize',14,'YLim',[-1 5]);
end
```

Disclaimer

This material was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the United States Department of Energy, nor Battelle, nor any of their employees, nor any jurisdiction or organization that has cooperated in the development of these materials, makes any warranty, express or implied, or assumes any legal liability or responsibility for the

accuracy, completeness, or usefulness or any information, apparatus, product, software, or process disclosed, or represents that its use would not infringe privately owned rights.

Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or Battelle Memorial Institute. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

PACIFIC NORTHWEST NATIONAL LABORATORY

operated by

BATTELLE

for the

UNITED STATES DEPARTMENT OF ENERGY

under Contract DE-AC05-76RL01830